A

Project Report

On

Steady state simulation of continuous stirred tank reactor (CSTR) system using Aspen Plus

Submitted by

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Under the guidance of

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CERTIFICATE

This is certified that the work contained in the thesis entitled **"Steady state simulation of continuous stirred tank reactor (CSTR) system using Aspen Plus"** *submitted by* ***Telagam Setty Maayedukondalu(111CH0504)****, has been carried out under my supervision and this work has not been submitted elsewhere for a degree.*

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ABSTRACT

This project work reports steady state simulation results of a continuous stirred tank reactor (CSTR) system using Aspen-plus simulation. The reaction, investigated in this work was production of ethyl benzene using ethylene and benzene as the reactants. Ethyl benzene, being one of the important raw materials in production of several industrially important chemicals, is often produced alongside with diethyl benzene as an undesired side product. In our simulation, this particular aspect has been examined to maximize the conversion of ethyl benzene from its reactants. Here, we have studied the effect of feed flow rate on steady state behaviour of CSTR and also obtained the optimum feed flow rate in order to maximize the conversion and yield with special consideration of consecutive reactions where one product was desired and another one was undesired. Since the effect of reactor temperature was always going to be crucial in this exothermic reaction mechanism, optimum values were evaluated. The optimum reactor volume was also found out from the simulation results. The optimum temperature was predicted to be 430 K and the optimum reactor volume was found to be 100 m^3. The optimum feed flow rates were 0.4 kmol/sec *w.r.t* benzene and 0.2 kmol/sec *w.r.t* ethylene. The maximum yield of ethyl benzene was predicted to be 49.75% *w.r.t* benzene and 99.9% *w.r.t* ethylene.

CONTENTS

List of Tables

List of Figures

NOTATIONS AND ABBREVIATIONS

B	Benzene
C_A	Concentration of component A (kmol/m^3)
C_B	Concentration of component B (kmol/m^3)
C_C	Concentration of component C (kmol/m^3)
C_D	Concentration of component D (kmol/m^3)
CSTR	Continuous stirred tank reactor
CUM	Cubic meter
DEB	Di-ethyl benzene
E	Ethylene
EB	Ethyl benzene
E_1 & E_2	Activation energy of reaction 1& 2, J/Kmol
F	Feed flow rate (kmol/s)
K_1 & K_2	Reaction rate constants, Kmol/s.m^3
P	Product flow rate (kmole/s)
PPM	Parts for million
T_R	Reactor temperature, K
X (B)	Conversion of benzene
X (E)	Conversion of ethylene
Y (EB/B)	Yield of ethyl benzene with respected to benzene
Y (EB/E)	Yield of ethyl benzene with respected to ethylene

CHAPTER 1

INTRODUCTION

This chapter highlights the importance of chemical reactors and also application of aspen plus in reactor design. It focuses on the uses of ethyl benzene which plays main role in the petrochemical industry as halfway in the production of styrene, the raw material for the production of polystyrene, a common plastic material. The background of the present thesis work is summarized along with the objectives.

1.1 PRELUDE

Reactions are usually the core of chemical processes in which comparatively low-cost raw materials are transformed into important products, useful to mankind in various forms [1-3]. Understanding the basics of chemical kinetics and thermodynamics are key before designing chemical reactors. Basically, kinetics and thermodynamics help in understanding how fast or slow the reaction is progressing and to what extent the reaction will progress. Designing chemical reactors is a tedious process and it requires plenty of expertise, starting from conceptualization to validation of data. Aspen-plus provides a platform in executing methods and predicts the effect of various parameters and variables reminiscent of a real-time system.

1.2 CHEMICAL REACTORS

The application of chemical reactors is very large and it is not only confined within the ambit of chemical industries but also petrochemical industries and any other process plants. Chemical kinetics and reactor design is the core to the understanding of the production of almost all chemicals. As mentioned in the aforesaid paragraph that designing chemical reactors is a tedious process and it requires plenty of expertise, starting from conceptualization to validation of data. Optimization of the best possible combination is in designing is the key. One particular route may yield a low reactor price but the handling of the chemicals; post production might be very expensive. The economics of the whole plant must be studied in great detail.

1.3 ASPEN PLUS

It is a process demonstrating instrument for steady-state simulation, design, performance, optimization and planning for chemicals, specialty chemicals, petrochemicals and metallurgy industries.

1.3.1 The Challenges

Understanding and Predicting Process Behavior [2]

The chemical process industries are beset with cases over fluctuating market conditions, government guidelines w.r.t environmental issues etc. However, there is no scope for any sluggishness and there has always been an effort to increase productivity with efficient mechanisms in place with improved economics of the plant and the country. When confronted with complicated situations like this, process engineers have little choice but to resort to strong and powerful software tools to answer them.

1.3.2 The Opportunity:

Maximizing Plant Performance and Enhancing Profitability [2]

Steady-state simulation is a prevailing process engineering tool that empowers engineers to simulate plant performance and examine their results quickly – exploiting the modern software and engineering technology to optimize plant performance and effectiveness.

1.3.3 The Solution:

Modeling and simulation involves deep understanding of the process starting from conceptualization to model development to its solution. It basically gives an idea to figure out what actually makes the process tick. Understanding the process and troubleshooting it as and when required makes process simulation such an attractive area to venture into. Aspen Plus is strong software, paving the way for giving ready-made solution to many challenging issues related to any process industry in a quick and legible way.

1.3.4 Benefits Offered by Aspen Plus [2]

Aspen Plus provides chemical process industries with considerable assistance throughout the manufacturing of a process starting from R&D through to engineering and into production. Using Aspen Plus, engineers can design, simulate and troubleshoot the process as and when the need arises.

1.4 ETHYL BENZENE

Ethylbenzene is a colorless liquid with a syrupy, gasoline odor. It is a small aromatic hydrocarbon. Ethylbenzene is manufactured through an alkylation of benzene. The alkylation can happen in vapor or in liquid phase and both alkylations use a zeolite or an aluminium chloride catalyst.

Uses of ethyl benzene:

As dissolvable: in inks, elastic cements, varnishes, and paints.

As an anti-knock agent: Ethylbenzene is supplementary to gas as an against thump specialists, significance it reduces motor thumping and acceleration the octane rating.

As recuperation of regular gas: Ethylbenzene may be infused into the ground.

Ethylbenzene: assumes critical part in the petrochemical business as a most of the way in the creation of styrene, the precursor to polystyrene, a typical plastic material. In 2012, more than 99% of ethylbenzene created was devoured in the generation of styrene.

Ethylbenzene is much of the time found in other made items, including pesticides, cellulose acetic acid derivation, and manufactured elastic.

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1.5 BACKGROUND OF PRESENT RESEARCH WORK

Ethylbenzene is an important raw material for the production of various other industrially important chemicals. Its industrial importance has attracted various researchers across the globe

to study their chemical synthesis using CSTR configuration. During synthesis it is almost imperative that some by-products will get produced from the stoichiometry. In production of ethylbenzene, di-ethylbenzene is produced as a by-product which is undesirable. The reactions involved are basically consecutive reactions. Presence of small amount of di-ethyl benzene generally leads to cross polymerization and requires to be avoided. In cases like this, reactor design becomes challenging simply because both yield and conversions need to be considered. These are the facts which prompted us to venture into studying ethylbenzene production in a continuous stirred tank reactor (CSTR) ensemble.

1.6 RESEARCH OBJECTIVES

- To study the effect of feed flow rate on steady state behavior of CSTR and also obtain optimum feed flow rate in order to maximize the conversion and yield (with special consideration of consecutive reactions) where one product is desired and another one is undesired.
- To study the effect of temperature on steady state behavior of CSTR and also obtain the optimum reactor temperature in order to maximize the conversion and yield with special consideration of exothermic reactions like preparation of ethyl benzene.
- To study effect of volume on steady state behavior of CSTR and also to obtain the optimum reactor volume in order to maximize the conversion and yield.
- To study steady state behavior of CSTRs especially when they are connected in series for the same reaction.

CHAPTER 2

LITERATURE REVIEW

2.1 INTRODUCTION

A synthetic reactor is a device utilized as a part of a substance procedure (plant) where concoction changes (responses) happen to deliver a particular item at an unequivocal generation rate, utilizing certain science. The reactor arrangement and its working conditions are chosen to accomplish certain destinations, for example, expanding the income of the methodology, and decreasing the era of contaminations, while fulfilling a few outlines and working constraints (security, controllability, accessibility of crude materials, and so forth.). For the most part, the execution of the compound reactor demonstrates a critical part in the operation and financial matters of the complete methodology since its operation bothers most different units all the while (partition units, utilities, and so on.) [1, 3].

2.2 ORGANIZATION OF CHEMICAL REACTIONS

Mainly chemical reactions are classified into two types; they are homogeneous reaction and heterogeneous reaction. Heterogeneous reactions further classified into four different types; they are fluid- fluid reactions, Non-catalytic gas-solid reactions, catalytic gas-solid reactions and catalytic gas-liquid-solid reactions.

The reactions occur between two immiscible phases i.e. Gas-liquid or liquid-liquid is called as fluid –fluid reactions. These types of reactions generally take place at the interface. The overall reaction rate depends on the miscibility of the reactant, available interface area and mass transfer rates.

The reactions like combustion, gasification of coal, and roasting of pyrites; which generally take place on the solid surface are called non-catalytic gas solid reactions. The reaction occurs when the gaseous reactants are transported to the interface, where it reacts with the solid reactant. The reaction rate depends on surface area and the mass transfer rate of the gaseous reactants.

The reactions in which both reactant and products are gaseous are called catalytic gas-solid reactions. Reactions occur at special catalytic sites present on the solid surface. Porous particles are generally used to provide large surface area to facilitate the reaction. The reaction rate depends on diffusion rate of reactant into the interior of the catalyst pore and diffusion of product out of the catalyst pore.

The reactions in which three states are involved i.e (solid, liquid and gases) are called catalytic gas –liquid-solid reaction. Here solid surface act as catalyst has a special reacting sites. Solid surface normally covered with liquid reactants and gaseous reactants are diffusion onto the catalytic site.

2.3 GENERAL DESCRIPTION AND REACTION TYPES

Chemical reactions relating to the chemical, petrochemical and oil industries are executed in distinct apparatus so-called reactors. There are distinct types of reactors projected to face exceptionally diverse operating circumstances, both in relationships of the nature of the chemical species involved(reactants and products of the reaction) and of the physical circumstances under which they operate.

In general, a chemical reactor needs to be able to carry out at least three functions:

- Offer the essential residence time for the reactants to complete the chemical reaction;
- Permit the needed heat exchange;
- To enable the chemical reaction, it brings all the phases into near contact.

Consequently, reactor categories range from huge measurement ceaseless reactors, similar to those embraced for synergist breaking responses, particularly for oil refineries, to gadgets of unobtrusive measurements, as spasmodic mixed reactors in which fine and optional science responses are performed. Additionally, there are reactors for advanced microelectronic applications and reactors of minuscule measurements (small scale reactors), intended for biomedical establishments or for in situ generation of greatly dangerous or perilous mixes. Converters and burners, reactant or generally, embraced for vitality generation can likewise be recorded among the reactors [3].

To classify a reactor, the quantity of stages in the reactor itself, whether there are unsettling frameworks and the method of operation (constant reactor, semi-nonstop or intermittent) crucial to be contemplated. It ought to additionally be noticed that most synthetic reactors are furnished with warmth trade mechanical assembly as outer coats or inward curls with a liquid coursing through them to go about as a warm vector to permit both warmth supply and evacuation [3-4].

2.4 DIFFERENT TYPE OF CHEMICAL REACTORS

2.4.1 BATCH REACTOR

The established bunch reactor is a splendidly blended vessel in which reactants are changed over to items throughout a clump cycle. All variables change rapidly with time. The reactants are charged into the vessel. Heat and/or impetus is added to launch response. Reactant fixations lessening and item focuses increment with time. Temperature or weight is controlled by coveted time direction. Bunch time is likewise an outline and working variable, which has a solid effect on profitability [1].

Temperature profiles are made so that change and yield targets are accomplished while not surpassing warmth exchange limit impediments. These ideal temperature profiles rely on upon the science. For instance, if the response is reversible and exothermic, the temperature profile may increase to a high temperature to get the responses going and afterward drop off with time to keep away from the decline in the compound balance consistent at high temperature. On the off chance that the response is reversible and endothermic, the temperature profile would ascend to the most elevated conceivable temperature as fast as could be allowed on the grounds that the synthetic harmony steady increments with temperature [1].

On the off chance that all the reactants are charged to the reactor, the reactant focuses are at first expansive, which implies that the response rate is high and the warmth exchange burden is high toward the start of the bunch cycle unless the temperature is kept low. The beginning high reactant fixation issue can be evaded by utilizing a "bolstered bunch reactor." Some material is at first charged to the reactor, yet the majority of the reactant is sustained over the span of the cluster cycle. This causes the volume of the fluid in the reactor to increment with time, so volume and in addition arrangements and temperatures are untouched fluctuating [1].

2.4.2 TUBULAR PLUG FLOW REACTOR

The real recognizing normal for tubular reactors is their conveyed parameter nature, that is, variables change with physical measurements and in addition with time. The traditional attachment stream reactor expect that the reactor vessel is tube shaped, that liquid streams down

the length of the reactor with a level speed profile, that no pivotal blending happens, and that no spiral angles exist in temperature or syntheses [1, 3].

The tubular reactor can be an unfilled vessel if no impetus is utilized. On the off chance that a strong impetus is needed, the vessel is pressed with impetus, either in a bed or inside tubes. The dynamic conduct of the reactor is fundamentally influenced by the vicinity of impetus in the reactor in light of the fact that the warm capacitance of the impetus is generally more prominent than that of the methodology liquid, especially if the framework is gas-stage. The temperatures of both the procedure liquid and the impetus change with time. Obviously, under unfaltering state conditions, the two temperatures are approach at any pivotal position [1, 4].

2.4.3 CONTINUOUS STIRRED-TANK REACTOR

The fluid in the reactor is thought to be flawlessly blended, that is, with no spiral, hub, or precise slopes in properties (temperature and arrangement). The item stream has a piece and a temperature that are precisely the same as the substance of the fluid all through the vessel. This is constantly genuine, both under consistent state conditions and progressively anytime [1].

This normal for a CSTR instantly creates a characteristic shortcoming of the CSTR kind of reactor, that is, the convergence of reactant in the vessel is the same as the amassing of reactant in the item. The amassing of reactant is contrarily identified with transformation [1].

2.4.3.1 There are several features of a CSTR that impact controllability:

1. A mixture of strategies and designs can be utilized for warmth exchange. Since warmth exchange is one of the important matters in reactor regulator, the CSTR is generally additional effortlessly organized than a tubular reactor. It is substantially hard to change the warmth evacuation down the length of a tubular reactor [1].

2. The temperature of the food has some impact on controllability; however it is a great deal less imperative in a CSTR than in a tubular reactor. In the event that warmth is being expelled from

the reactor, a bolster that is at a lower temperature than the temperature in the reactor will lessen the warmth exchange necessities [1, 3].

3. Change is the part of a reactant that is nourished to the reactor that responds in the reactor. The level of transformation in a CSTR has an exceptionally critical effect on its solidness and controllability. A high transformation implies a little reactant fixation in the reactor vessel, so there is little "fuel" accessible to allow a reactor runaway [1].

Then again, a low transformation implies that there is a lot of reactant accessible to respond. In the event that the response is exothermic and irreversible, a reactor temperature runaway can all the more effortlessly happen in a CSTR working with low reactant change than in one working with high reactant transformation. Notwithstanding influencing reactant focus, the outline change influences reactor size. Low transformation implies a littler reactor. This little reactor has less warmth exchange zone if an outer coat or an inside curl is utilized, which has a negative effect on controllability [1, 4].

2.4.3.2 Characteristics of Continuous stirred tank

Run at unfaltering express, the stream rate in must equivalent the mass stream rates out, generally the tank will flood or go unfilled (transient state).

The feed accept a uniform organization all through the reactor; way out stream has the same concentration as in the tank.

The reaction rate associated with the final (yield) concentration.

Reactor outfitted with an impeller to guarantee fitting blending.

Dividing the volume of the tank by the normal volumetric stream rate through the tank gives the living arrangement time, or the normal measure of time a discrete amount of reagent spends inside

2.4.4 DESIGN EQUATION FOR CONTINUOUS STIRRED TANK REACTOR (CSTR)

CONSECUTIVE REACTIONS

Reactor configuration gets to be all the more fortifying when yield and in addition change must be considered. One normal circumstance in which this emerges is when there are successive irreversible responses, for example, the accompanying:

$$A + B \rightarrow C \qquad \rightarrow (2.1)$$

$$C + B \rightarrow D \qquad \rightarrow (2.2)$$

The wanted item is C. The undesired item is D. There are numerous critical mechanical illustrations of this sort: chlorination, oxidation, and nitration of an assortment of hydrocarbons. The particular response rates for the first and second responses are K1 and K2, separately [1, 3].

The "conversion" of reactant A is defined as

Conversion of A

= (moles A fed - moles A leaving reactor)/ (moles A fed) → (2.3)

There are several ways to define "yield" (or "selectivity") of the desired product C. One is on the basis of the amount of A fed. The other is on the basis of the amount of A that has reacted.

Yield 1 = (moles C produced) / (moles A fed) → (2.4)

Yield 2 = (moles C produced) / (moles A reacted) → (2.5)

The desirable product C is produced by the first reaction whose rate depends on the concentrations of A and B in the reactor. But C is consumed by the second reaction whose rate depends on the concentrations of C and B in the reactor [1][8].

$$R_C = -K_1C_AC_B+K_2C_CC_B$$

$$= -C_AC_BK_{01}e^{-(E_1/RT_R)} +C_CC_BK_{02}e^{-(E_2/RT_R)} \qquad \rightarrow (2.6)$$

$$R_D = -K_2 C_C C_B$$

$$= -C_C C_B K_{02} e^{-(E_2/RT_R)} \rightarrow (2.7)$$

Where the reaction rates $\mathbf{R_C}$ and $\mathbf{R_D}$ are rates of consumption.

It is evident that the best approach to outline this reactor is to keep the concentration of C and B little to keep the second response rate little. This infers that a vast abundance of reactant A ought to be utilized as a part of the reactor, which will weaken the C and B concentration. It will likewise help to drive the first response in view of the huge estimation of C_A regardless of the little estimation of C_B. With this plan, the every pass transformation of A will be little, however the yield of C every mole of A responded will be huge.

The drawback of this configuration is that the overabundance A absolute necessity be recuperated and reused, which implies high capital and vitality costs. Be that as it may, the subsequent change in the yield of C is regularly definitely justified even despite the included expense. This is especially genuine when the undesirable item D is lethal, destructive, and unstable or an ecological toxin that is hard to discard. Natural and wellbeing concerns have pushed the outlines of numerous compound courses of action to incorporate a few expansive reuse streams so that the yields of alluring items are expanded and the yields of undesirable items are diminished. These reuse streams build the trouble of the plant wide control issue [1].

There are four components, so four component balances can be written.

Component A balance (kmol A/s):

$$F_{A0}C_{A0} = FC_A + V_R K_1 C_A C_B \rightarrow (2.8)$$

Components B balance (kmol B/s):

$$F_{B0}C_{B0} = FC_B + V_R (K_1 C_A C_B + K_2 C_C C_B) \rightarrow (2.9)$$

Components C balance (kmol C/s):

$$0 = FC_C + V_R (-K_1 C_A C_B + K_2 C_C C_B) \rightarrow (2.10)$$

Component D balance (kmol D/s):

$$0 = FC_D - V_R K_2 C_C C_B \rightarrow (2.11)$$

The assumption of constant liquid densities means the volumetric flowrate of the reactor effluent F is the sum of the two volumetric feed flowrates [1, 7].

CHAPTER 3

SIMULATION WORK

In this chapter the simulation methodology is discussed.

3.1 Aspen plus software

Aspen plus v 8.4 was used for the simulation work.

3.2 ASPEN PLUS REACTOR MODEL

RCSTR simulator was used for this work.

3.3 PROPERTY METHOD

CHAO-SEADER thermodynamic model was used as the property method.

3.4 STEADY STATE SIMULATION

3.4.1 Chemical Kinetics

The specific chemistry used to understand the steady state behavior of CSTR and demonstrate the use of Aspen Plus is the reaction of ethylene (E) with benzene (B) to form the favored product ethylbenzene (EB). There is a repeated reaction that produces an unwanted product di-ethylbenzene (DEB). A third reaction association's benzene and diethyl benzene to form ethylbenzene [1]:

$$E + B \rightarrow EB \quad \rightarrow (3.1)$$

$$E + EB \rightarrow DEB \quad \rightarrow (3.2)$$

$$DEB + B \rightarrow 2EB \quad \rightarrow (3.3)$$

The reactions follow in the liquid phase and are assumed to be irreversible. The reaction rates of the three reactions are assumed to be those given here:

$$R_1 = (C_E)\,(C_B)\,(1.528\times10^6)\,e^{(-71130000)/RT} \quad \rightarrow (3.4)$$

$$R_2 = (C_E)(C_{EB})(2.778\times10^3)e^{(-83680000)/RT} \quad \rightarrow (3.5)$$

$$R_3 = (C_{DEB})(C_B)(0.4167)e^{(-62760000)/RT} \quad \rightarrow (3.6)$$

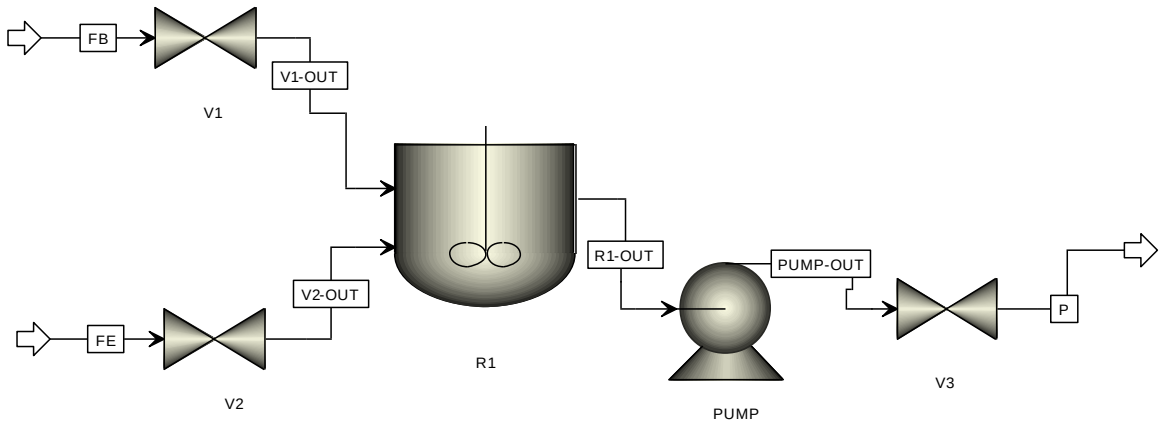
The units of R are kmol s^{-1} m^{-3}. Concentrations have units of kmol/m^3. Activation energies have units of J/kmol. Temperature is in degrees Kelvin [1].

C_E is the concentration of ethylene; C_B is the concentration of benzene,

C_{EB} is the concentration of ethyl benzene; C_{DEB} is the concentration of di-ethylbenzene.

3.5 SIMULATION SETUP

Figure 3.1 Schematic representation of the continuous stirred tank reactor (CSTR)



By carefully analyzing the above chemical reactions and rate kinetics we would have the following conclusion about feed flow rate, reactor temperature and reactor volume.

3.4.1 Effect of feed flow rate

The feed flow rate of benzene must be greater than the feed flow rate of ethylene in order to lower formation of undesired product i.e. di-ethyl benzene. Increasing the feed flow rate of benzene also has negative impacts such as increasing separation cost which is added to the production cost i.e. minimizing the profit margin.

The solution for above problem is optimizing the feed flow rate by using the aspen plus by keeping the one of the feed flowrate constant and varying the other one.

3.4.2Effect of reactor temperature

By comparing the enthalpies of above reaction, the enthalpy of undesired product is greater than the enthalpy of desired product which mean, that the increasing the reactor temperature favors the formation of undesired product more than the desired product. So it is necessary to maintain the optimum reactor temperature in order to maximize the performances.

3.4.3 Effect of reactor volume

Reactor provides sufficient residence time to the reactants where the reactants are converted into products. In case of exothermic reaction heat removal is necessary in that case reactor provides sufficient reactor area for jacketed cooling. Increasing the reactor volume provides better cooling but aggregate the residence time and capital cost. Decreasing the reactor volume may lead to the process become uncontrollable and it lead to the formation of undesired product.

CHAPTER 4

RESULTS AND DISCUSSION

4.1 OPTIMIZATION OF FEED FLOW RATE

First we do the optimization of feed flow, for this we need to fix other quantities like reaction temperature and reactor volume. From the literature review we have a good idea about reactor temperature and reactor volume which may or may not be optimum values.

Let's take the feed flow rate of ethylene is F (E) = 0.2 kmol/s, Reactor temperature T (K) = 430 K

And the Reactor volume V = 100 (cum)

By varying the benzene flow rate F (B) = 0.1, 0.2, 0.3, 0.4, 0.5, and 0.6 (kmol/s), run the simulation and obtained stream results was tabulated as follows.

Table 4.1: Comparison between the feed flow rate and product flow rate

Feed flow rate (kmol/s)		Product flow rate (kmol/s)			
Benzene(F)	Ethylene(F)	Benzene(P)	Ethylene(P)	Ethyl benzene	Di-ethylbenzene
0.1	0.2	0.002	0.098	0.095	0.003
0.2	0.2	0.022	0.021	0.178	0.001
0.3	0.2	0.108	0.008	0.192	<0.001
0.4	0.2	0.207	0.007	0.193	<0.001
0.5	0.2	0.307	0.007	0.193	<0.001
0.6	0.2	0.407	0.007	0.193	<0.001

Table 4.2: Comparison between the feed flow rate and product mole fraction

Feed flow rate (kmol/s)		Product mole fraction			
Benzene(F)	Ethylene(F)	Benzene(P)	Ethylene(P)	Ethyl benzene	Di-ethylbenzene
0.1	0.2	0.008	0.496	0.48	0.016
0.2	0.2	0.098	0.095	0.804	0.004
0.3	0.2	0.351	0.026	0.622	0.000598
0.4	0.2	0.509	0.017	0.474	0.00024
0.5	0.2	0.606	0.014	0.381	0.00013
0.6	0.2	0.671	0.012	0.318	0.000082

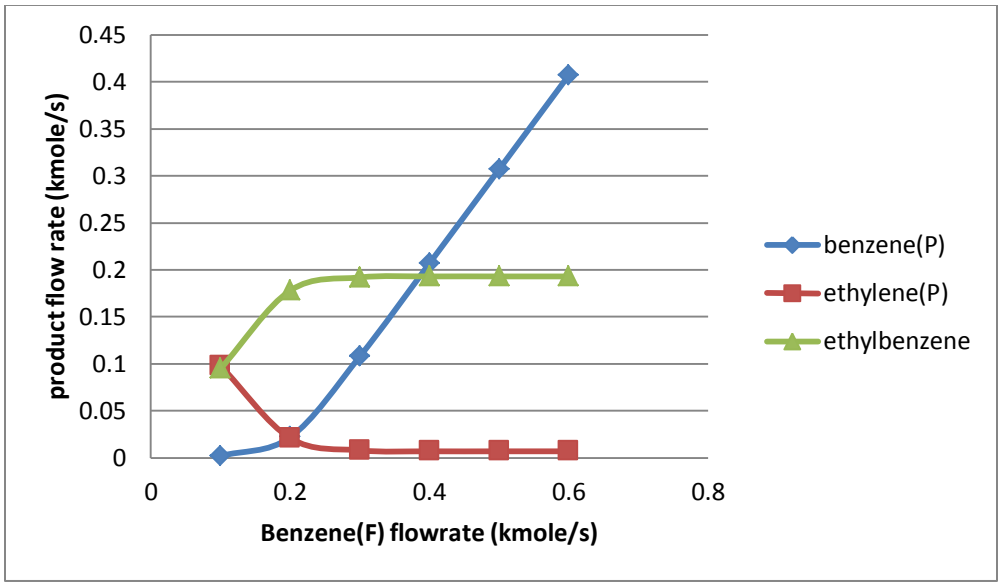


Figure 4.1: Feed flow rate vs product flow rate

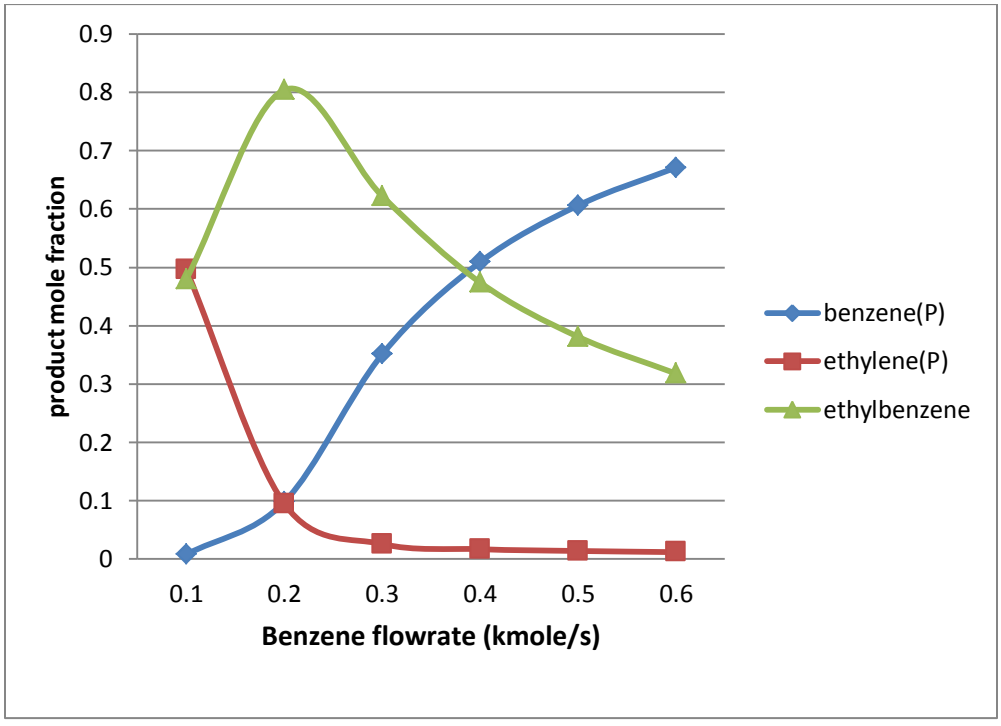


Figure 4.2: Flow rate vs product mole fraction

Table 4.3: Comparison between benzene flow rate and concentration of di-ethyl benzene (ppm)

Benzene(F) Flow rate (kmol/s)	Di-ethyl benzene Mole fraction(ppm)
0.1	160000
0.2	4000
0.3	598
0.4	240
0.5	130
0.6	82

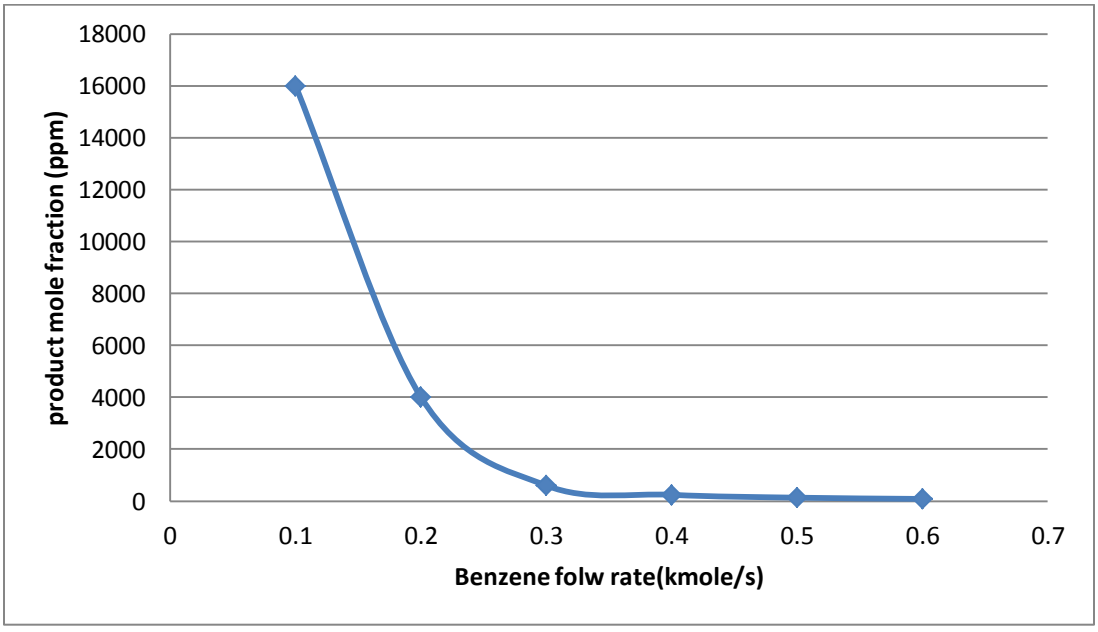


Figure 4.3: Benzene flow rate (kmol/s) vs concentration of DEB (ppm)

4.1.1 Inferences from the tables and graphs

By carefully analyzing the tables and graphs we would have the following conclusions. Increasing the benzene feed flow rate up to 0.4 kmol/s lead to the maximization of product formation then after further increasing the feed flow have no effect on product formation instead increasing the separation cost. So optimum combination of feed flow benzene is F (B) = 0.4 kmol/s and ethylene is F (E) = 0.2 kmol/s.

4.2 OPTIMIZATION OF REACTOR TEMPERATURE

Similarly like above here we fixing the feed flow rate of benzene F (B) =0.4 and ethylene

F (E) =0.2 kmol/s, reactor volume V (cum) = 100.

By varying the reactor temperature T (k) = 410,420,430,440,450,460,470 and 480, run the simulation and obtained stream results were tabulated as follows.

Table 4.4: Comparison between reactor temperature and product flow rate

Temperature	Product flow rate (kmol/sec)			
T(K)	benzene(P)	ethylene(P)	ethylbenzene	di-ethylbenzene
410	0.216	0.016	0.184	<0.001
420	0.211	0.01	0.189	<0.001
430	0.207	0.007	0.193	<0.001
440	0.205	0.005	0.195	<0.001
450	0.203	0.003	0.197	<0.001
460	0.202	0.002	0.198	<0.001
470	0.202	0.002	0.198	<0.001
480	0.201	0.001	0.199	<0.001

Table: 4.5 Comparison between reactor temperature and product mole fraction

Temperature T(K)	Product mole fraction			
	benzene(P)	ethylene(P)	ethylbenzene	DEB(ppm)
410	0.519	0.038	0.442	173
420	0.513	0.025	0.452	208
430	0.509	0.017	0.474	240
440	0.506	0.011	0.482	271
450	0.504	0.008	0.488	300
460	0.503	0.005	0.491	328
470	0.502	0.004	0.494	355
480	0.502	0.003	0.495	383

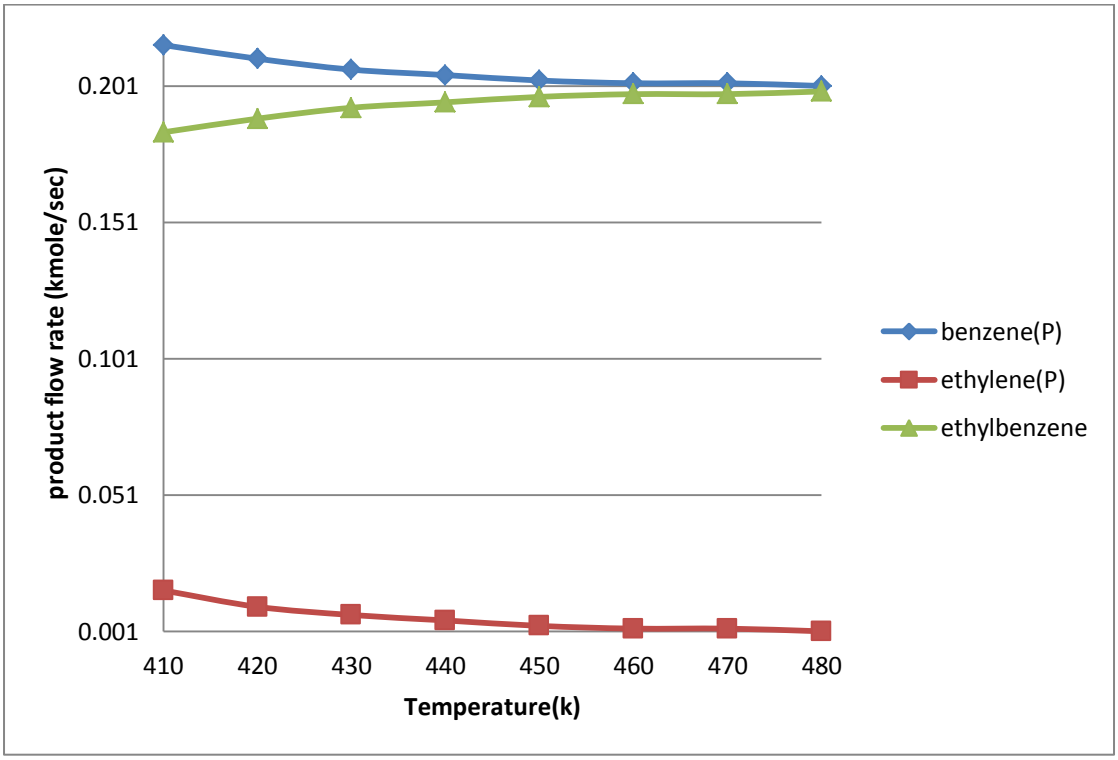


Figure 4.4: Reactor temperature vs product flow rate

Table: 4.6 Comparison between reactor temperature and concentration of di-ethyl benzene (ppm)

Reactor Temperature T(K)	Di-ethyl benzene mole fraction (ppm)
410	173
420	208
430	240
440	271
450	300
460	328
470	355
480	383

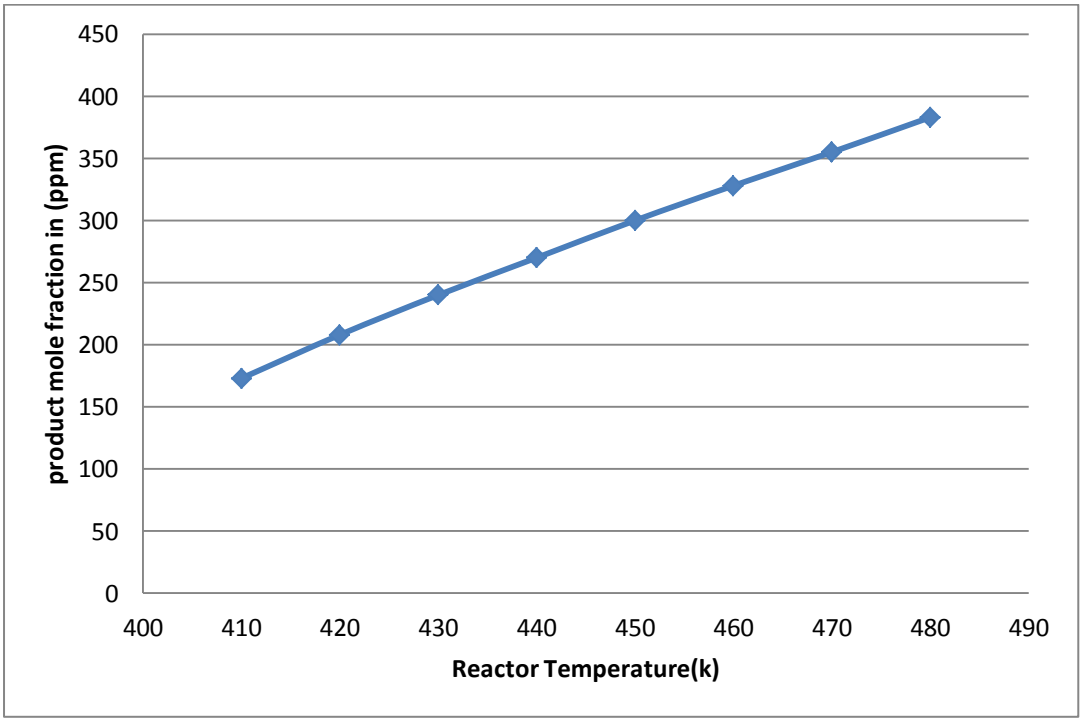


Figure 4.5: Reactor temperature vs product mole fraction (DEB)

4.2.1 Inferences from the graphs and tables

By carefully analyzing tables and graphs we would have following conclusions.

By increasing the reactor temperature favours the product formation i.e ethyl benzene and further increasing the temperature may also favours formation of undesired product i.e di-ethyl benzene. So the optimum temperature of the reactor is T (k) = 430.

4.3 OPTIMIZATION OF REACTOR VOLUME

Similarly like above here we fixing the feed flow rate of benzene F (B) =0.4 and

Ethylene F (E) =0.2 kmol/s, reactor temperature T (K) = 100.

By varying the reactor volume V = 60, 80, 100, 120 and 140, run the simulation and obtained stream result were tabulated as follows.

Table 4.7: Comparison between reactor volume and product flow rate

Reactor volume (cum)	Product flow rate (kmol/sec)			
	benzene(P)	ethylene(P)	ethylbenzene	di-ethylbenzene
60	0.211	0.011	0.189	<0.001
80	0.209	0.009	0.191	<0.001
100	0.207	0.007	0.193	<0.001
120	0.206	0.006	0.194	<0.001
140	0.205	0.005	0.195	<0.001

Table 4.8: Comparison between reactor volume and product mole fraction

Reactor volume (cum)	Product mole fraction		
	benzene(P)	ethylene(P)	ethylbenzene
60	0.514	0.027	0.4519
80	0.511	0.021	0.468
100	0.509	0.017	0.474
120	0.507	0.014	0.478
140	0.506	0.012	0.481

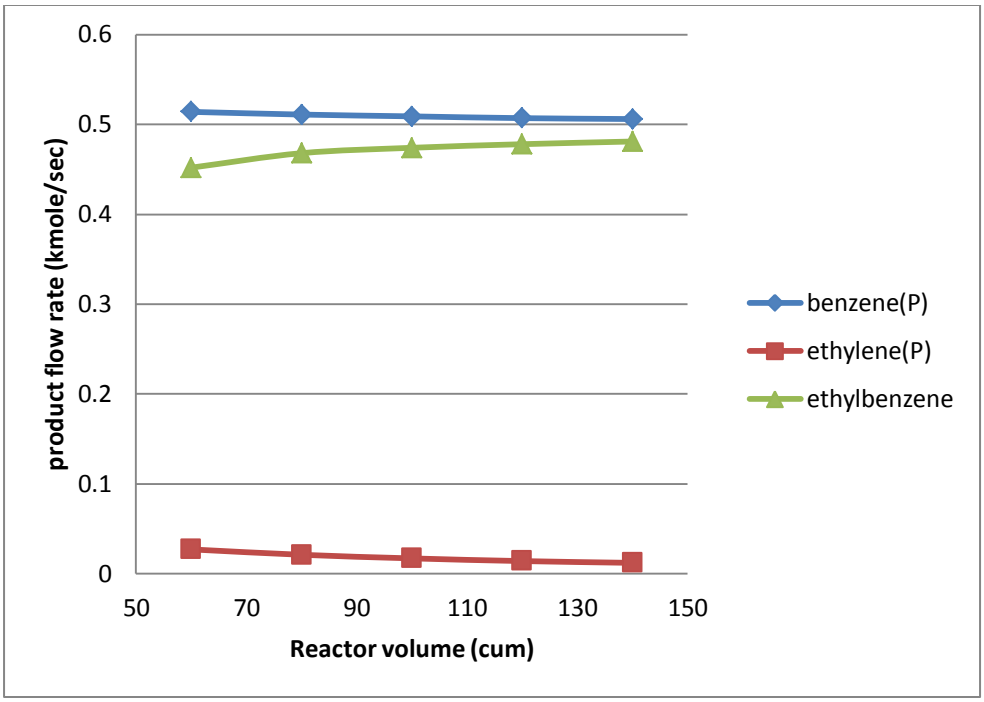


Figure 4.6: Reactor volume vs product flow rate

Table 4.9: Comparison of reactor volume with di-ethyl benzene flow rate

Reactor volume (cum)	Di-ethylbenzene flow rate (kmol/s)
60	223
80	233
100	240
120	245
140	248

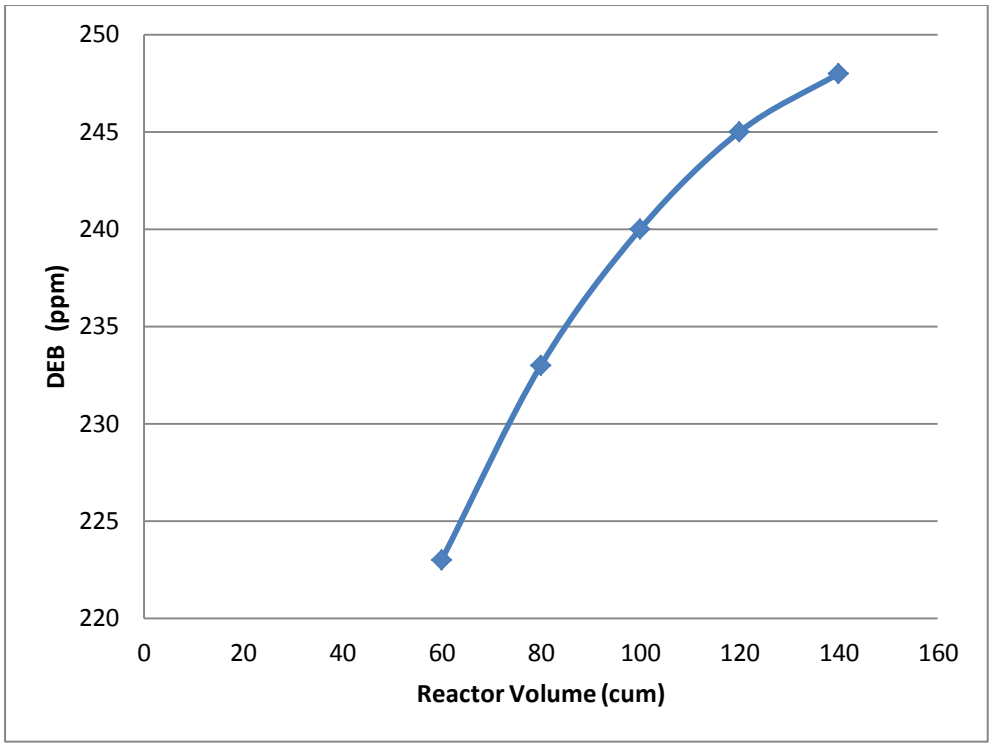


Figure 4.7: Reactor volume vs DEB (ppm)

4.3.1 Inferences from graphs and tables

By carefully analyzing tables and graphs we would have following conclusions.

Increasing the reactor volume favours the formation of both the desired product and undesired product simultaneously. Increasing the reactor volume is not also economically feasible. Since it is exothermic reaction we need to maintain minimum reactor volume for jacketed cooling so optimum reactor temperature is T (K) = 430.

From the above date we would have the optimum values for feed flow, reactor temperature and reactor volume. Putting this optimum values in aspen plus and run the simulation and obtain the stream table which is show below.

Table: 4.10 Stream results for steady state simulation

preparation of ethylbenzene								
Stream ID		FB	FE	P	PUMP-OUT	R1-OUT	V1-OUT	V2-OUT
Temperature	K	298.0	298.0	430.4	430.3	430.0	298.2	372.2
Pressure	N/sqm	1.51988E+6	1.51988E+6	1.21590E+6	1.51988E+6	1.01325E+6	1.01325E+6	1.01325E+6
Vapor Frac		0.000	1.000	0.000	0.000	0.000	0.000	0.000
Mole Flow	kmol/sec	0.400	0.200	0.407	0.407	0.407	0.400	0.200
Mass Flow	kg/sec	31.245	5.611	36.856	36.856	36.856	31.245	5.611
Volume Flow	cum/sec	0.036	0.296	0.051	0.051	0.051	0.036	0.026
Enthalpy	MMkcal/hr	17.029	8.902	15.241	15.241	15.211	17.029	8.902
Mole Flow	kmol/sec							
B		0.400		0.207	0.207	0.207	0.400	
E			0.200	0.007	0.007	0.007		0.200
EB				0.193	0.193	0.193		
DEB				< 0.001	< 0.001	< 0.001		
Mole Frac								
B		1.000		0.509	0.509	0.509	1.000	
E			1.000	0.017	0.017	0.017		1.000
EB				0.474	0.474	0.474		
DEB				240 PPM	240 PPM	240 PPM		

4.4 STEADY STATE SIMULATION FOR CSTRs in SERIES

4.1 Flow sheet for CSTRs in series

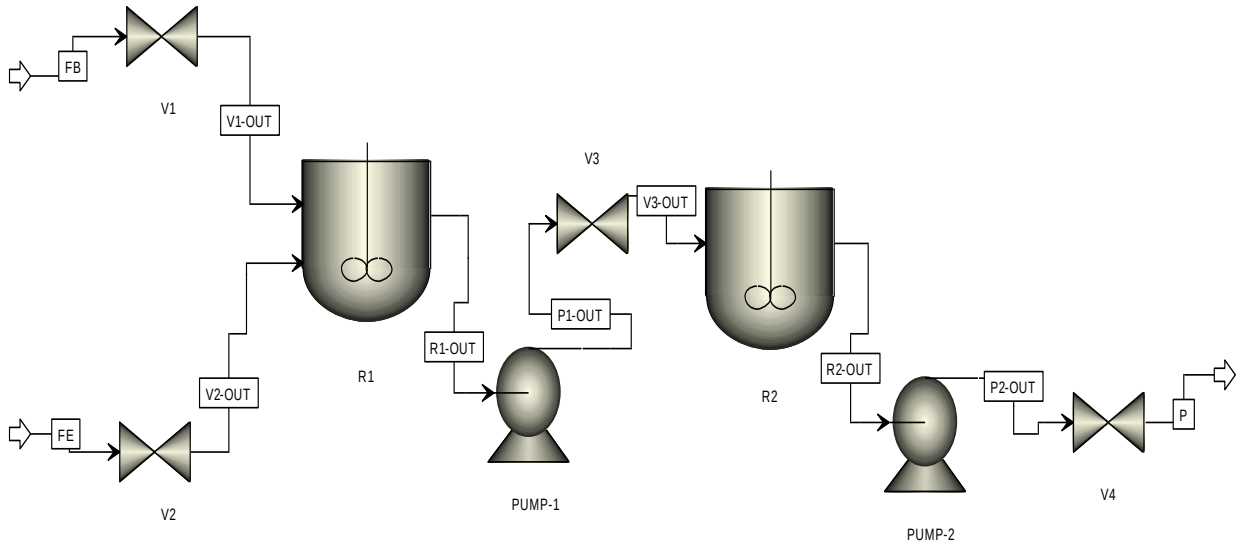


Figure 4.8: schematic flow sheet for series CSTR

The optimum size ratio of two CSTRs in series is found to be dependent on the reaction kinetics and on the level of the conversion.

For reactions with first order kinetics, equal-size CSTRs are the best. For reactions with order greater than one, the smaller size CSTR should be followed by the large one and for reactions with order less than one the larger size CSTR should be followed by one with the smaller size.

4.5 SIMULATION FOR OPTIMUM SIZE RATIO

Here we are taking two reactors instead of single reactor having combined volume equal to volume of single reactor. Use the same optimum values like feed flow, reactor temperature are used in previous case. Run the simulation for various combination of reactor volume like ((10,90) ,(20,80) , (30,70) , (40, 60) , (50,50) , (60,40) , (70,30) , (80,20) , (90,10)) and obtained stream results tableted as follows.

Table 4.11: Comparison between reactor volumes and product flow rate

Reactor volume (cum)		Flow rare (kmol/s) from R1 & R2					
R1	R2	R1(B)	R1(E)	R1(EB)	R2(B)	R2(E)	R2(EB)
10	90	0.249	0.049	0.151	0.202	0.002	0.198
20	80	0.229	0.029	0.171	0.201	0.001	0.199
30	70	0.221	0.021	0.179	0.201	0.001	0.199
40	60	0.216	0.016	0.184	0.201	0.001	0.199
50	50	0.213	0.013	0.187	0.201	0.001	0.199
60	40	0.211	0.011	0.189	0.201	0.001	0.199
70	30	0.21	0.01	0.19	0.201	0.001	0.199
80	20	0.209	0.009	0.191	0.201	0.001	0.198
90	10	0.208	0.008	0.192	0.202	0.002	0.198

Table 4.12: Comparison between reactor volumes and product mole from R1 &R2

Reactor vol (cum)		Mole fraction from R1 & R2 and DEB in PPM (parts per million)							
R1	R2	R1(B)	R1(E)	R1(EB)	R1(DEB)	R2(B)	R2(E)	R2(EB)	R2(DEB)
10	90	0.554	0.109	0.337	111	0.503	0.005	0.493	186
20	80	0.534	0.067	0.399	162	0.502	0.003	0.495	210
30	70	0.525	0.049	0.426	188	0.501	0.003	0.496	224
40	60	0.519	0.038	0.442	204	0.501	0.002	0.496	232
50	50	0.516	0.032	0.452	215	0.501	0.002	0.496	238
60	40	0.514	0.027	0.459	223	0.501	0.002	0.496	242
70	30	0.512	0.024	0.464	229	0.502	0.003	0.496	245
80	20	0.511	0.021	0.468	233	0.502	0.003	0.495	247
90	10	0.51	0.019	0.472	237	0.503	0.005	0.492	248

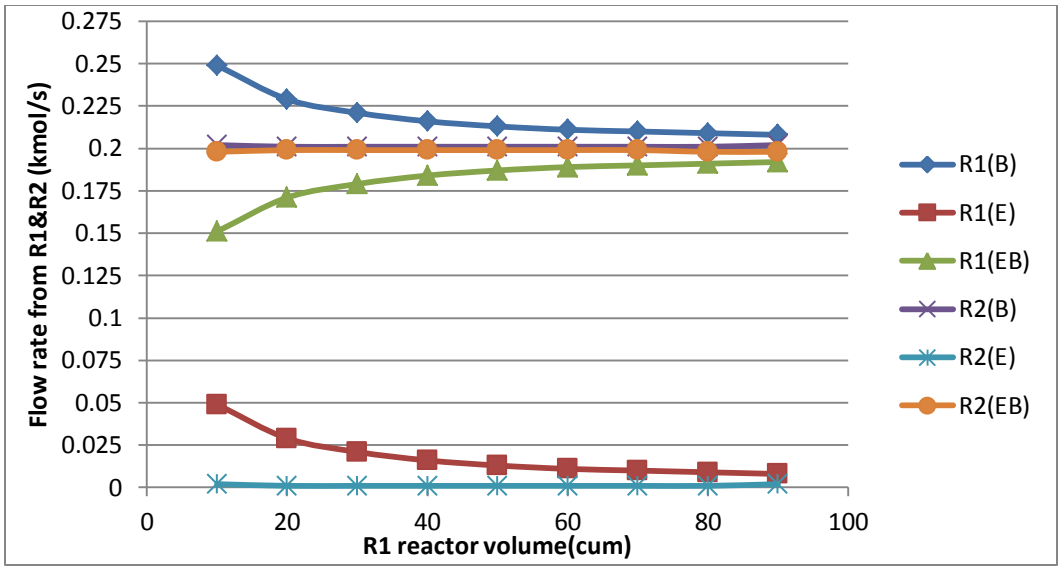


Figure 4.9: R1 and product flow rate curves

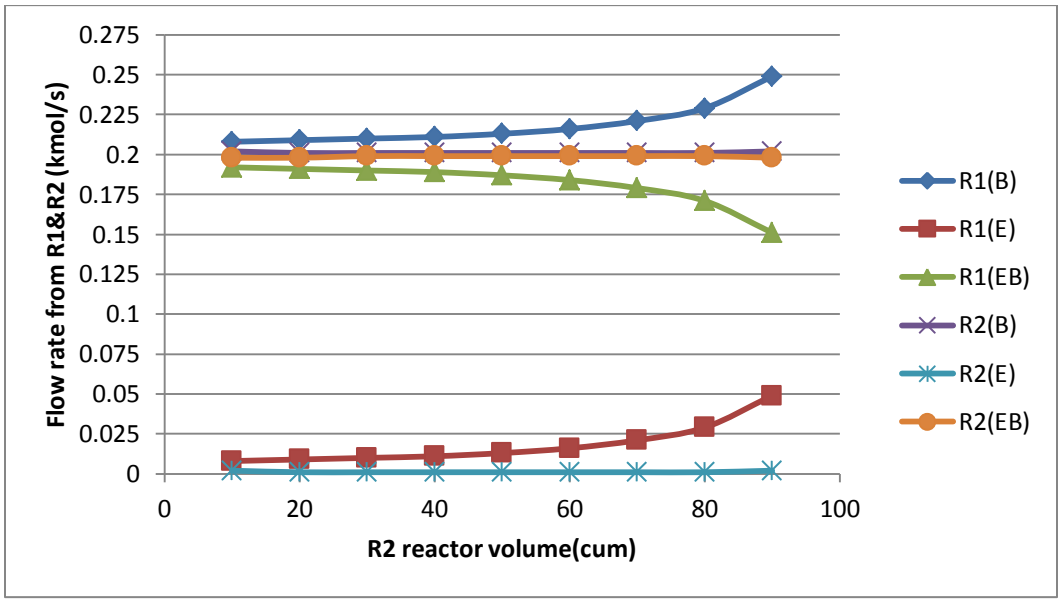


Figure 4.10: R2 and product flow rate curves

Table 4.13: Comparison between R1 vol (cum) & formation of DEB (ppm) in R1 & R2

R1 Vol (cum)	R1(DEB)(ppm)	R2(DEB)(ppm)
10	111	186
20	162	210
30	188	224
40	204	232
50	215	238
60	223	242
70	229	245
80	233	247
90	237	248

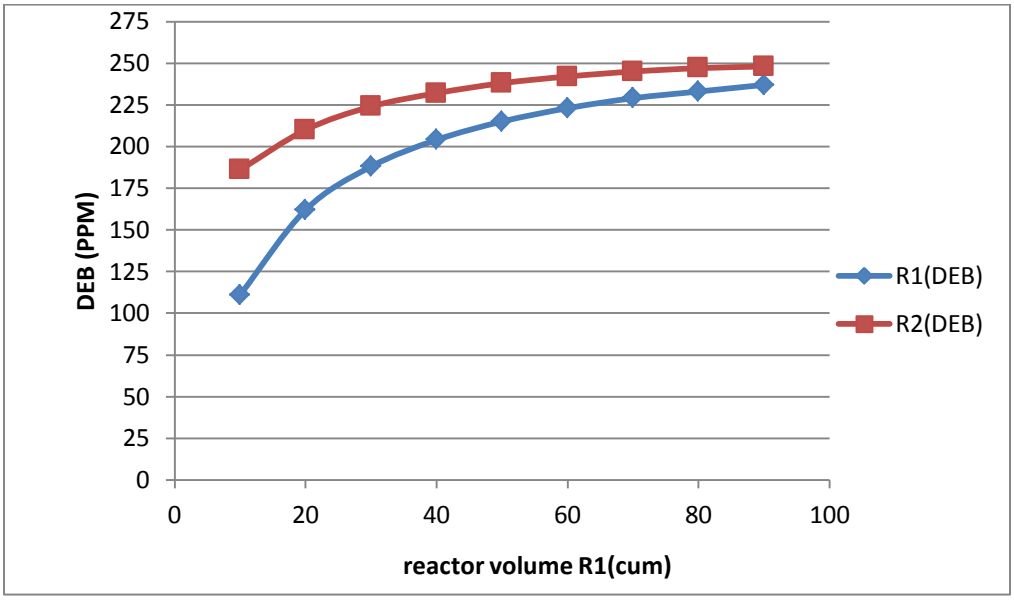


Figure 4.11: Plot between reactor volume R1 vs DEB (ppm)

Table 4.14: Comparison between R2 vol (cum) & formation of DEB (ppm) in R1 & R2

R2 Vol (cum)	R1(DEB)(ppm)	R2(DEB)(ppm)
90	111	186
80	162	210
70	188	224
60	204	232
50	215	238
40	223	242
30	229	245
20	233	247
10	237	248

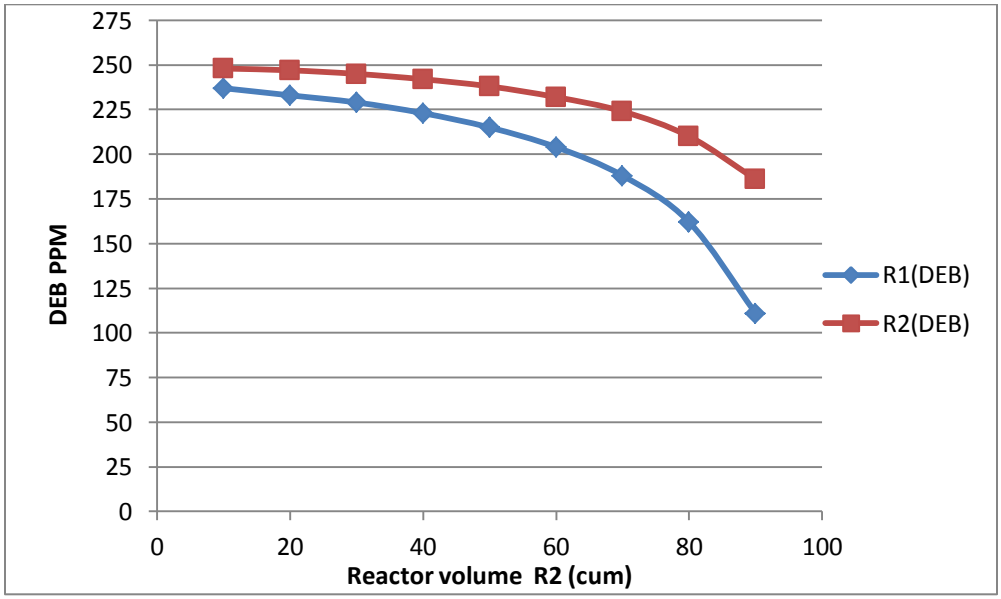


Figure 4.12: Plot between reactor volumes R2 vs DEB (ppm)

4.5.1 Inferences from plots and graphs

By carefully analyzing the data tables and graphs we would have following conclusions.

Initially we are started simulation with the reactor volume R1 =10 & R2=90 and with increasing reactor volume R1 we can observe increasing of production formation. Further increasing the reactor volume beyond certain limit i.e R1=40(cum), it favours the formation of undesired product i.e di-ethyl benzene. So optimum reactor volume combination is R1 = 40 & R2 =60.

Put all this values and the run simulation we will get following stream table.

Table 4.15: Stream results for CSTRs in series

preparation of ethylbenzene											
Stream ID		FB	FE	P	P1-OUT	P2-OUT	R1-OUT	R2-OUT	V1-OUT	V2-OUT	V3-OUT
Temperature	K	298.0	298.0	430.4	431.0	430.3	430.0	430.0	298.2	372.2	212.8
Pressure	N/sqm	1.51988E+6	1.51988E+6	1.21590E+6	2.53313E+6	1.51988E+6	1.01325E+6	1.01325E+6	1.01325E+6	1.01325E+6	10.000
Vapor Frac		0.000	1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.874
Mole Flow	kmol/sec	0.400	0.200	0.401	0.416	0.401	0.416	0.401	0.400	0.200	0.416
Mass Flow	kg/sec	31.245	5.611	36.856	36.856	36.856	36.856	36.856	31.245	5.611	36.856
Volume Flow	cum/sec	0.036	0.296	0.051	0.051	0.051	0.051	0.051	0.036	0.026	64337.983
Enthalpy	MMkcal/hr	17.029	8.902	14.683	16.151	14.683	16.062	14.654	17.029	8.902	16.151
Mole Flow	kmol/sec										
B		0.400		0.201	0.216	0.201	0.216	0.201	0.400		0.216
E			0.200	0.001	0.016	0.001	0.016	0.001		0.200	0.016
EB				0.199	0.184	0.199	0.184	0.199			0.184
DEB				< 0.001	< 0.001	< 0.001	< 0.001	< 0.001			< 0.001
Mole Frac											
B		1.000		0.501	0.519	0.501	0.519	0.501	1.000		0.519
E			1.000	0.002	0.038	0.002	0.038	0.002		1.000	0.038
EB				0.496	0.442	0.496	0.442	0.496			0.442
DEB				232 PPM	204 PPM	232 PPM	204 PPM	232 PPM			204 PPM

Table 4.16: Comparison between reactor temperature vs conversion & yield

T(k)	X(B)	X(E)	Y(EB/B)	Y(EB/E)
410	0.46	0.92	0.46	0.92
420	0.4725	0.95	0.4725	0.945
430	0.4825	0.965	0.4825	0.965
440	0.4875	0.975	0.4875	0.975
450	0.4925	0.985	0.4925	0.985
460	0.495	0.99	0.495	0.99
470	0.495	0.99	0.495	0.99
480	0.4975	0.995	0.4975	0.995

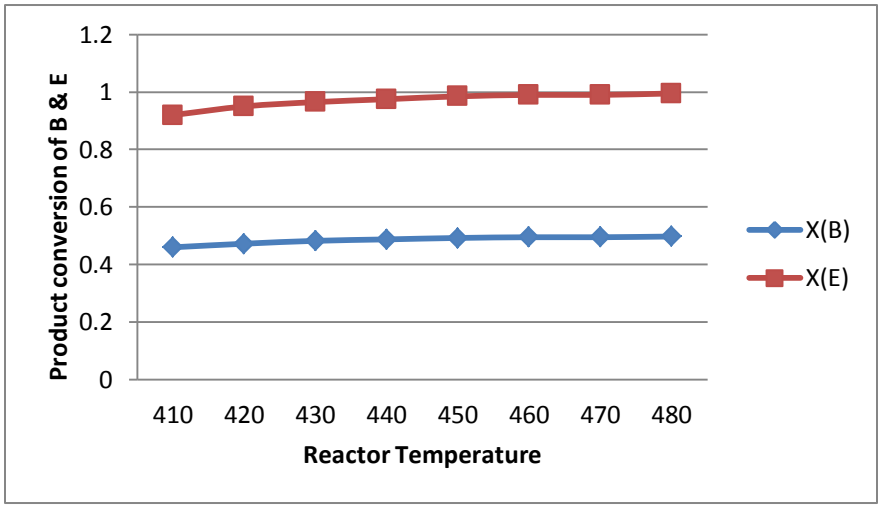


Figure 4.13: Plot between reactor temperature vs conversion of B & E

Table 4.17: Comparison between reactor volume and conversion & yield

Reactor volume(cum)	X(B)	X(E)	Y(EB/B)	Y(EB/E)
60	0.4725	0.945	0.4725	0.945
80	0.4775	0.955	0.4775	0.955
100	0.4825	0.965	0.4825	0.965
120	0.485	0.97	0.485	0.97
140	0.4875	0.975	0.4875	0.975

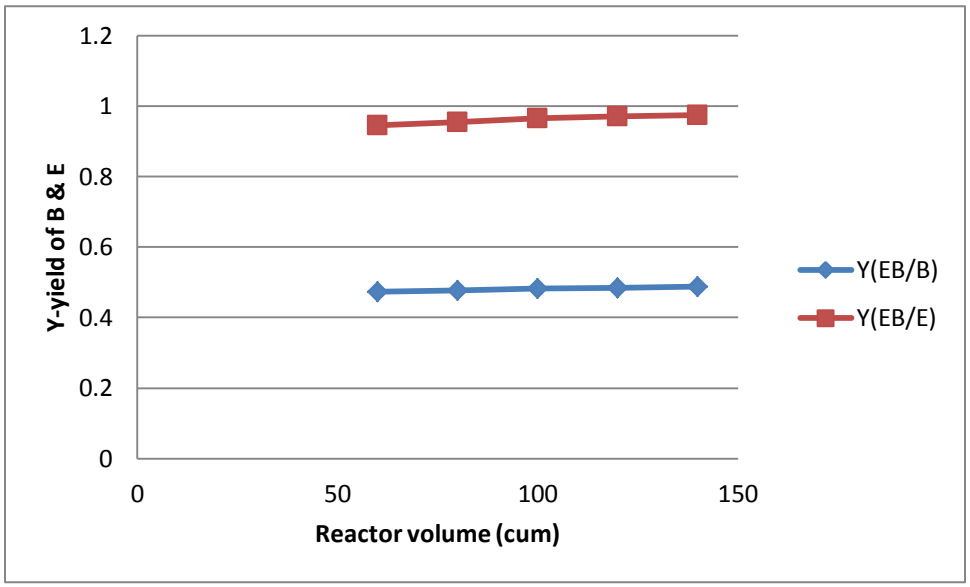


Figure 4.14: Plot between reactor volume vs Yield of B & E

Table 4.18: Comparison between feed flow rate vs conversion & yield

Benzene(F)(kmol/s)	X(B)	X(E)	Y(EB/B)	Y(EB/E)
0.1	0.98	0.51	0.98	0.9312
0.2	0.89	0.895	0.89	0.9944
0.3	0.64	0.96	0.64	0.999
0.4	0.4825	0.965	0.4825	0.999
0.5	0.386	0.965	0.386	0.999
0.6	0.322	0.965	0.322	0.999

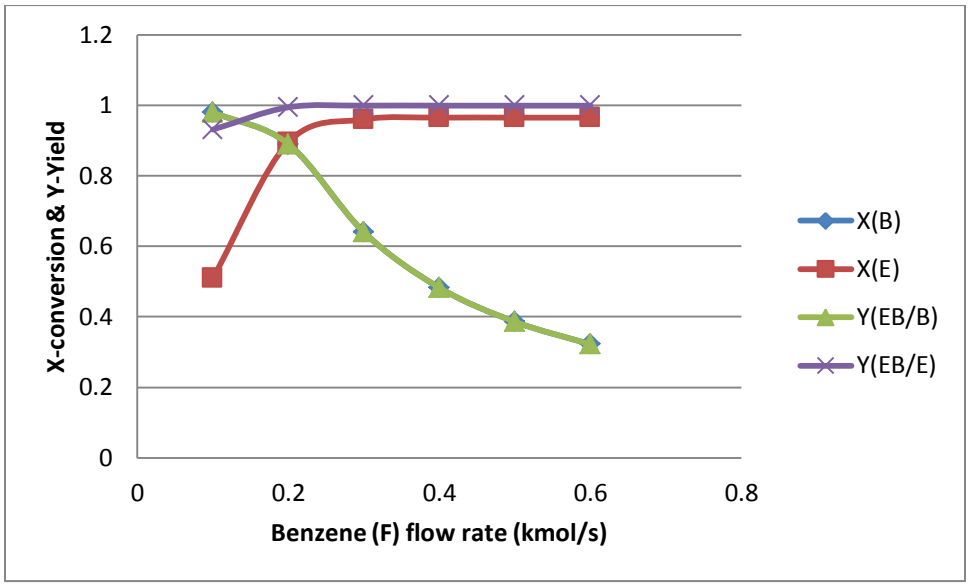


Figure 4.15: Plot between feed flow rate vs conversion & yield

Inferences:

By carefully analyzing the above table and graphs we would have the following conclusions.

At optimum reactor temperature (T = 430K), reactor volume (V = 100) and feed flow rate (kmol/s) (F (B) =0.4, F (E) =0.2) the reaction has maximum conversion and yield.

Conversion and yield values for single tank reactor are

Conversion of benzene X (B) = 48.5%

Conversion of ethylene X (E) = 96.5%

Yield of ethyl benzene Y (EB/B) = 48.25%

Yield of ethyl benzene Y (EB/E) = 99.9%

Conversion and yield values for series CSTR reactor are

Conversion of benzene X (B) = 49.75%

Conversion of ethylene X (E) = 99.5%

Yield of ethyl benzene Y (EB/B) = 49.75%

Yield of ethyl benzene Y (EB/E) = 99.99%

By comparing the two models we have following results

Conversion of benzene is X (B) increased by 2.58%

Conversion of ethylene is X (E) increased by 3.1%

Yield of ethyl benzene Y (EB/B) is increased by 3.1%

Yield of ethyl benzene Y (EB/E) is increased by 3.61 %

DISCUSSION

For single tank reactor at optimum reactor temperature T=430(k), reactor volume V=100 (cum)

And feed flow rate i.e benzene F (B) =0.4 & ethylene F (E) 0.2 kmol/s, the conversion of benzene and ethylene were found to be 48.5% and 96.5%. The yield of ethyl benzene Y (EB/B)

And Y (EB/E) was found to be 48.25% & 96.5%.

By replacing single reactor with series reactors whose sum of the volumes is equal to the volume of the single reactor, the performance of the reaction can be enhanced.

For series CSTR at the same reaction conditions i.e temperature and feed flow the conversion of benzene and ethylene were found to be 49.75% and 99.5%. The yield of ethyl benzene Y (EB/B) and Y (EB/E) was found to be 49.75% & 99.9%.

By comparing the two reactor models i.e single tank vs series reactor system we would have following conclusion.

The conversion of benzene is increased by 2.58% and ethylene is increased by 3.1%.

The yield of ethyl benzene Y (EB/B) is increased by 3.1% and yield of ethyl benzene Y (EB/E) is increased by 3.61%.

CHAPTER 5

CONCLUSION AND FUTURE WORK

This project work reports steady state simulation results of a continuous stirred tank reactor (CSTR) system using Aspen-plus simulation. The reaction, investigated in this work was production of ethyl benzene using ethylene and benzene as the reactants. Ethyl benzene, being one of the important raw materials in production of several industrially important chemicals, is often produced alongside with diethyl benzene as an undesired side product.

In our simulation, this particular aspect has been examined to maximize the conversion of ethyl benzene from its reactants. Here, we have studied the effect of feed flow rate on steady state behaviour of CSTR and also obtained the optimum feed flow rate in order to maximize the conversion and yield with special consideration of consecutive reactions where one product was desired and another one was undesired.

Since the effect of reactor temperature was always going to be crucial in this exothermic reaction mechanism, optimum values were evaluated. The optimum reactor volume was also found out from the simulation results.

The optimum temperature was predicted to be 430 K and the optimum reactor volume was found to be 100 m^3. The optimum feed flow rates were 0.4 kmol/sec *w.r.t* benzene and 0.2 kmol/sec *w.r.t* ethylene.

The maximum yield of ethyl benzene was predicted to be 49.75% *w.r.t* benzene and 99.9% *w.r.t* ethylene.

As a continuation of this work, it can be extended in studying the dynamic simulation aspects with various controlling mechanisms in place and to figure out controller parameters and settings. Similarly, different reactor volumes (variable hold-ups) may also be used in series to study their affect in overall conversion of this reaction and optimize the variables.

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